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Cometary Atmospheres:
Modeling the Spatial Distribution
of Observed Neutral Radicals

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16. Abstract New data for the spatial distribution of cometary C_2 are presented. A re-compilation of the Haser scale lengths for C_2 and CN resolves the previously held anomalous drop of the C_2/CN ratio for heliocentric distances larger than 1 AU. Clues to the source of cometary C_2 have been found through fitting the sunward-antisunward brightness profiles with the Monte Carlo particle-trajectory model. A source (parent) lifetime of 3.1×10^4 seconds has been found, and an ejection speed for C_2 radicals upon dissociation of the parent(s) of $\sim 0.5 \text{ km s}^{-1}$ has been calculated.			
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Program of Research for the Second Quarter

Research activities during the second quarter have primarily involved the completion and submission for publication of a paper on C_2 and CN in comets written in collaboration with A. H. Delsemme.

C_2 and CN in Comets

Attached to this report is a preliminary version of the paper completed this quarter and submitted to the Astrophysical Journal which deals with the spatial distributions and inferred production rates of the C_2 and CN radicals in comets.

The principal contents of the paper briefly enumerated are:

- (1) new observations of C_2 brightness profiles,
- (2) compilation of C_2 and CN scale lengths from previously published data, as well as their heliocentric distance dependences,
- (3) re-evaluation of published filter photometry with the new scale length data which resolves the previously held anomalous C_2 -to-CN production ratio's behavior with increasing heliocentric distance; and
- (4) an analysis of sunward and antisunward C_2 profiles with the Monte Carlo particle-trajectory model which implies a total source (parent) lifetime of 3.1×10^4 s at 1 AU and an excess photolysis-energy ejection speed of 0.5 km s^{-1} for C_2 radicals.

In addition to the submission of this paper for publication, these results were presented at the Baltimore meeting of the Division of Planetary Sciences at the end of October (Combi and Delsemme 1985). Also presented at this meeting was an exhibit on the general effort at AER in the area of modeling cometary atmospheres which contained preliminary results of the effects of elastic collisions on the spatial distributions of cometary radicals (Combi and Smyth 1985).

Program of Research for the Third Quarter

Research activities during the third quarter will focus on evaluation of available observations of the spatial distributions of the C_3 and OH radicals in comets.

References

Combi, M. R., and A. H. Delsemme, 1985: Bull. AAS 17, 689.

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NEUTRAL COMETARY ATMOSPHERES V

C₂ AND CN IN COMETS

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ABSTRACT

Brightness profiles of C_2 in comets Bennett (1970II) and Kohoutek (1973XII) are presented. Model analysis of these profiles yields radial Haser scale lengths for production and destruction of C_2 which, when combined with other scale length determinations in the literature, are shown to vary as the square of the heliocentric distance. This is consistent with photochemical production and destruction. Also presented is an updated compilation of CN scale lengths which shows that the mean parent scale length law varies as $r^{+1.5}$. A re-analysis of published cometary photometry, using the new scale length laws, yields a C_2 -to-CN ratio which is independent of heliocentric distance. The previously documented drop-off in C_2 production rate relative to other neutral species for heliocentric distances larger than ~ 1.5 AU was a simple artifact of the previously assumed scale length variations.

Analysis of the sunward-tailward distortion of the brightness profiles with a Monte Carlo particle-trajectory model shows that C_2 is released from its parent molecule with an ejection speed of about 0.5 km s^{-1} , owing to the excess photolysis energy. This result also implies that the photochemical lifetimes for the C_2 parent and C_2 respectively are 3.1×10^4 seconds and 1.2×10^5 seconds at 1 AU.

I. INTRODUCTION

The Swan system ($d^3\Pi_g - a^3\Pi_u$) of C_2 dominates the emission spectra of most comets at visible wavelengths. Furthermore, the detection of C_2 along with C_3 has suggested the possible presence of hydrocarbons in comets. Thus, although it is really one of the minor components of the comae of comets, C_2 has been the subject of considerable study. Despite this effort, though, there are still many unanswered questions regarding both its production mechanism(s) and its detailed excitation mechanism.

Although it has been long accepted that the excitation of C_2 emission bands is through resonance fluorescence with solar light (Swings 1941), and much progress has been made in modeling the observed Swan band intensity distribution (Arpigny 1966; Krishna Swamy and O'Dell, 1977, 1979; A'Hearn 1978; Lambert and Danks 1983), fundamental unknowns still exist. The ground state of C_2 is $x^1\Sigma_g^+$; therefore, intercombination transitions must play an important role. Krishna Swamy and O'Dell (1979) had assumed an intercombination transition of $a^3\Pi_u - x^1\Sigma_g^+$ with a rate, $A \sim 10^{-3} \text{ s}^{-1}$, which was later found to be consistent with the Mulliken ($d^1\Sigma_u^+ - x^1\Sigma_g^+$) system intensity discovered by A'Hearn and Feldman (1980). However, more recent studies by Johnson et al. (1983) and Lambert and Danks (1983) do not favor this ad hoc assumption and point to the likely importance of intercombination transitions involving excited triplet states.

A principal method for studying the production and destruction mechanisms for observed cometary radicals has been the observation and model analysis of their spatial distributions. Modeling has generally been done with Haser's (1957) model which provides radial scale lengths for production and decay. These can be related to true photochemical lifetimes if the ejection velocity

of the daughter radical and the expansion velocity of parent molecule are known (Combi and Delsemme 1980a, hereafter referred to as Paper I).

We present here revised sunward and antisunward brightness profiles of the C_2 (0-0) band of the Swan system in Comet Bennett (1970II), and a pair of profiles in Comet Kohoutek (1973XII). Laser model scale lengths determined for these profiles are then compared with those found by other investigators to examine their heliocentric distance dependence. The separate sunward and antisunward profiles are then analyzed with the Monte Carlo particle-trajectory model as described in Paper I and used similarly by Combi (1980) for pairs of CN profiles. Since the solar radiation pressure on C_2 radicals can be calculated, the sunward-antisunward distortion can be modeled to deduce photochemical lifetimes from the spatial distribution. The newly revised C_2 scale length laws and those determined from an updated compilation of CN observations are then used to re-examine the production rates as determined from filtered photometry. Finally, possible sources of C_2 are discussed in the light of the other results presented in this paper.

II. MODELING THE SPATIAL DISTRIBUTIONS OF NEUTRAL RADICALS

There are active today three major broadly-defined approaches to modeling the spatial distributions of neutral cometary species. The traditional method is, of course, that put forth in the model of Haser (1957), which considers observed daughter radicals to be produced at a constant rate from a source of exponentially decaying parent molecules streaming radially from a point source nucleus. The radicals continue to move radially and decay exponentially themselves. The two decay times are related to scale lengths by the assumed radial velocity. A closed form expression for the column density can be written in terms of simple integrals of modified Bessel functions. The two scale lengths give the model enough parameter flexibility such that it can be fitted to almost any observed radial brightness profile. Unfortunately, early attempts to identify suspected parent molecules by comparing observed scale lengths with photochemical lifetimes (Potter and DelDuca 1964, Delsemme and Moreau 1973) generally found cometary scale lengths to be too short to be explainable by photochemistry alone.

At this point, two other possible sources of dissociation or ionization of parent molecules had been suggested. These were gas phase chemistry (Aiken 1974 and Oppenheimer 1975), particularly fast ion-molecule reactions, and an internal ionization source created by the interaction between solar wind flow through the cometary plasma (Ip and Mendis 1975, 1976a, 1976b, 1977) in combination with chemistry. These ideas evolved through large complicated chemistry models having >100 species and >1000 gas phase and photochemical reactions (see Huebner et al. 1982, and Mitchell et al. 1981) finally into multi-fluid chemical-dynamic models which address the feedback of photochemistry, and radiative transfer on the energy balance of the inner coma (Marconi

and Mendis 1982, 1983, and Huebner and Keady 1983). The former of these two schemes, a one-dimensional chemistry model, has been adopted by Cochran (1982, 1985) to analyze observations of cometary radicals. This model calculates the non-equilibrium chemistry occurring in a single fluid parcel of cometary gas moving radially away from the nucleus' surface at a constant velocity and expanding, of course, as r^2 . Results for CN (Cochran 1982) and C_2 (Cochran 1985) are apparently consistent with photochemical production of these two species. In fact, the earlier results of this type of chemical model generally underproduced radicals which could not be produced by a one- or two-step photodissociation (Giguere and Huebner 1978).

A third general approach to the question of modeling the spatial distribution of cometary radicals was developed simultaneously with the chemical models and is based on the principal weakness of the simple Haser model. That is, when a radical or atom is produced during the photodissociation of its immediate parent molecule or radical, there is in general some excess energy which is divided between the internal energy of the fragments (i.e., rotationally, vibrationally, or electronically excited states) and translational energy. This translational energy can impart extra non-radial velocities to the newly created fragments which are of the same order or even much larger than the typical outflow velocities of the parent molecules of 0.3 to 1.0 km/s (Whipple 1980, Delsemme 1982), e.g., 1.2-1.5 km/s for OH from H_2O , ~20 km/s for H from H_2O , ~8 km/s for H from OH, ~1 km/s for CN from HCN, 3-7 km/s for C and O from CO and CO_2 (Huebner and Carpenter 1979, Festou 1981b).

The vectorial model (Festou 1978, Festou et al. 1979, Festou 1981a, 1981b) addressed the non-radial radical velocities in a way similar to Haser's model, i.e., in terms of a closed-form multiple-integral expression for the space or column density of an observed radical. Festou successfully

applied the vectorial model to the distributions of OH as well as H in the inner ($<10^5$ km) coma. The vectorial model requires at least a triple numerical integration to calculate the column density for single parent outflow and daughter ejection velocities.

Work by the authors (Combi 1979, 1980, Combi and Delsemme 1980a, 1980b) addressed the same question of non-radial radical velocities in two different ways. One was the Average Random Walk Model (ARWM), which was based on a simple geometric re-interpretation of Haser model scale lengths as radial projections of true non-radial scale lengths. The second was the introduction of a Monte Carlo model which simulates the actual photochemical kinetics by calculating explicit particle trajectories for many individual radicals. We successfully applied the ARWM to show that 16 symmetric brightness profiles (i.e., average of sunward-antisunward pairs) of CN in Comets Bennett (1970II) and West (1976VI) could be explained by the photodissociation of cometary HCN but not CH_3CN . Combi (1980) went on to explain the observed distortion in the sunward-antisunward pairs of CN brightness profiles in terms of the expected excess velocity imparted to CN during the photodissociation of HCN combined with the radiation pressure force using the Monte Carlo model.

The principal qualitative results found in both studies of non-radial radical motion were that the use of the Haser model resulted in a measurement, in fact, of a radial projection of the true scale length, and thus would always give smaller values than one might suspect from photochemical lifetimes, and that the effect of non-radial motion is both measurable and important. Furthermore, the cases of H and OH from H_2O and CN from HCN can in fact be understood in terms of purely (but geometrically correct) photochemical models, for generally large comets with supposedly well developed collision zones and ionospheres.

The single fluid one-dimensional chemistry models (e.g., Huebner and Giguere 1978, Mitchell et al. 1981, and Cochran 1982, 1985a) of course cannot easily address the problem of non-radial motion. Huebner and Keady (1983) have used our ARWM to approximate the transition from collision dominated flow to free flow in vacuum in their multi-fluid chemical dynamic models. They are currently working on a more fundamental treatment of the transition region (Huebner 1984). Finally, a two-dimensional multi-fluid model (one fluid for each observed species) that treats this transition zone in a proper way would be required to attack the problem of the radiation pressure distortion which is quite apparent for C_2 and CN for heliocentric distances < 1 AU.

Let us enumerate a few "points" regarding these various modeling efforts:

(1) That chemical reactions (especially the fast ion-neutral reactions) occur in the inner regions ($r < 1000$ km) of comets with large gas production rates for heliocentric distances < 1 AU is not questioned. The rates for the reactions involving particular species may well dominate photochemical rates in the inner coma regions. A major reshuffling of ion species may in fact occur, and the special case of observed $C(^1D)$ may be produced by dissociative recombination. However, the situation is complicated by the fact that a gas parcel only spends on the order of 1000 seconds in this region, and all the gas phase chemistry must occur in that time scale.

(2) Photochemical reaction rates vary from 10^{-4} to 10^{-6} s^{-1} . However, since the rates depend only on the square of the heliocentric distance and in some cases on the heliocentric velocity, they have no time constraint and should generally dominate in the long run.

(3) The impressively large base of information gathered by A'Hearn and his collaborators over the last 12 years in the form of photometric observations of the major visible radicals and dust has demonstrated that there are

no systematic compositional differences between the gas composition of the comae of large and small gas producing comets. This corresponds to gas production rates (and collision zone radii) varying by well over two orders of magnitude. The only consistently anomalous behavior has been that of the apparent fall-off in the C_2 abundance relative to all other species for heliocentric distances larger than 1.2 AU, and even this behavior seems to be independent of the comets' gas production rates (A'Hearn and Cowan 1980, A'Hearn 1982; see Section IV of this paper). The uniformity seems also to be evident in the growing base of ultraviolet data, especially from IUE (again with the exception of $C(^1D)$, Weaver et al. 1983, Feldman 1982).

(4) Even the results of Cochran (1982, 1985a), which used a single-fluid one-dimensional constant-outflow-velocity non-equilibrium chemistry model, point to photodissociation of parent molecules as by far the dominant source of the observed radical species.

(5) The simple single-fluid constant-outflow-velocity chemistry models are clearly inappropriate outside the collision zone. Here, exothermic non-thermal non-radial velocities and radiation pressure dominate the kinematics and either photodissociation, photoionization, or charge exchange impact with the solar wind dominate the radical production and decay processes.

(6) In the case of negligible impact by gas phase chemistry in this type of chemistry model, the density distribution of a radical should be virtually "identically reproduced" by a sum of either simple Haser models for the case of several single step photodissociations or at worst some type of multiple step grandparent-parent model as introduced by Malaise (1966). For example, Cochran (1985b) has recently fitted Haser models to observed C_2 , C_3

and CN profiles which had been previously analyzed with a 1-D chemistry model (Cochran 1982, 1985a).

(7) A major weakness of almost all modeling efforts is the fact that the principal shaping factor of the outer radical coma (i.e., the daughter scale length region $\sim 1-2 \times 10^5$ km) may in fact be the sporadic activity of the nucleus' vaporization. This was suggested some time ago by Malaise (1970) and was borne out by the measured Haser scale lengths for CN decay determined for Comets Bennett (1970II) and West (1976VI) (Combi and Delsemme 1980b). Figure 1 shows the variation of the two Haser scale lengths for observed CN brightness profiles. We have added points from Combi (1978), Cochran (1982), Delsemme and Combi (1983) and Johnson et al. (1984) to our original data. Although the variation of the parent scale lengths is not inconsistent with a simple r^2 law (owing to the large amount of scatter), the best power law fit is actually $\propto r^{1.5}$. On the other hand, we found no measurable trend in the Haser scale length for CN decay as a function of heliocentric distance as we had for the Haser scale length for decay of the CN parent (HCN). Rather, we found a fairly random distribution of values generally greater than 10^5 seconds. Simply put, this means that whereas a steady-state vaporization rate for time scales $< 10^4$ seconds may make it possible to identify parent molecule decay rates (or at least Haser scale lengths or source region sizes), either sporadic or periodic variations in the vaporization rate on time scales of $1-5 \times 10^5$ seconds may make it at least very difficult to model full observed brightness distributions. It should also be mentioned here that Cucchiarro and Malaise (1982) and Keller and Meier (1980) have attempted some models with time dependent outbursts in production rate to explain observed spatial distributions.

(8) Finally, the results of a chemical model run depend critically on many (nearly half) poorly known rate constants, and on the initial assumed composition of the nucleus' volatile mix (which is exactly what is unknown). The problem, of course, cannot be uniquely inverted even if all of the rate constants are precisely known. The agreement of the model profiles with observations is a necessary but not a sufficient condition for having the correct nuclear mix. Furthermore, some of the dominant photolytic rates used in these models are approximations derived from Haser model fits to observed brightness profiles.

In conclusion, since there has yet to be demonstrated a reasonable case for the production of any of the principally observed neutral cometary species - with the possible exception of $C(^1D)$ - by gas phase chemical reactions, it seems reasonable to choose some combination (or sum) of the exospheric photochemical models with which to attempt to understand the observations of the spatial distributions of neutral cometary species. A method we (Combi and Delsemme 1980a, 1980b, Combi 1980) have used still remains quite viable. This is to use the Haser model, realizing that the scale lengths may have no direct physical meaning (even for pure photochemistry) to characterize the spatial extent and heliocentric distance dependence of the source region. From this point, one can then move on to the ARWM interpretation of the scale lengths, and/or to explicit modeling with the Monte Carlo particle-trajectory models which can handle radiation pressure, collisions, velocity distributions and time dependencies as necessary.

Note that the simplest version of the particle-trajectory model, i.e., with non-radial ejection of photodissociated radicals, is fundamentally equivalent to the vectorial model (Festou 1981a). Also, even though neither the vectorial nor the particle-trajectory models are as directly invertible as

is Haser's, we are still left with only a handful of parameters, such as lifetimes and velocities, to specify, and we do not have to pre-specify the identity of a proposed parent but simply find the best-fit lifetimes and velocities for a given data set.

III. BRIGHTNESS PROFILES OF C_2

The brightness profiles of C_2 (0-0) presented here were determined from microdensitometer scans of spectrograms of Comet Bennett (1970II) and Comet Kohoutek (1973XII). The details regarding the observations and the principal data reduction have been discussed at length in earlier papers for both the Toledo plates of Comet Bennett (Delsemme and Combi 1979, Combi and Delsemme 1980b - Paper II) and the Lick plates of Comet Kohoutek (Delsemme and Combi 1983 - Paper IV), and will not be pursued further in this paper. Also see Delsemme and Combi (1979) for a discussion of the earlier C_2 profiles deduced from these plates of Comet Bennett by Delsemme and Moreau (1973). A systematic error in the original data reduction by Delsemme and Moreau, due to unsuspected vignetting in the spectrograph, was the reason for re-analyzing the CN data in Paper II and the C_2 data in this paper. We had cautioned in Paper II that a revision for the original C_2 scale lengths (similar to that for CN) was also likely. Relevant information concerning comet parameters for each observation are given in Table 1. The brightness profiles are shown in Figures 2 through 5. As noted in the figure captions, the profiles are exactly sunward and anti-sunward for the Bennett plates but are 51° from the true projected radius vector for the Kohoutek plate.

Parent and daughter scale lengths were determined with Haser's (1957) model using the same non-linear least squares method as in Paper II (also see Combi 1979) for the average symmetric profiles and are listed as part of Table 2. Also listed in Table 2 is a compilation of other measured Haser scale lengths determined for C_2 profiles in different comets from whole brightness profile observations only. Newburn and Spinrad (1984) have computed Haser model parent scale lengths for C_2 , C_3 , and CN from two-point spectrophotometry

of five different comets. They determined column densities within a 4 arc second diameter aperture centered on the nucleus and displaced 17 1/2 and 35 arc seconds from the nucleus. From the nucleus value and one displaced point, they determined a parent scale length and a production rate. In order to do this, they had to assume the value for the daughter scale lengths as adopted by A'Hearn (1982) from our earlier papers (Delsemme and Moreau 1973, and Paper II). In a few cases, they determined scale lengths using each displaced point in combination with the nucleus values, and differences up to a factor of 2 resulted. When using entire brightness profiles, both scale lengths can be determined with uncertainties of only 10 to 25%, so we will limit our study to this type of data (see Table 2 for references). Figures 6a and b show the variation with the comet's heliocentric distance of the C₂ parent and the C₂ radial Haser scale length, respectively. Simple power law fits to the data imply the following expressions for the C₂ parent and C₂ scale lengths:

$$\gamma_H(C_2 \text{ parent}) = 1.6 \times 10^4 r_H^{2.0 \pm .3} \text{ km}$$

$$\gamma_H(C_2) = 1.1 \times 10^5 r_H^{2.0 \pm .3} \text{ km} .$$

It is worth noting here that if we include the C₂ parent scale lengths determined by Newburn and Spinrad, the overall power law fit is not changed much, although their data do deviate much more from the mean power law. This is also true when comparing their CN results with the results from whole profiles (Figure 1).

IV. THE PRODUCTION RATES OF C_2 AND CN IN COMETS

A'Hearn, Thurber and Millis (1977, hereafter ATM), have published an extensive set of filter photometric observations of C_2 , C_3 and CN over a wide range of heliocentric distance for Comet West (1976VI). In Paper II we had re-reduced their CN data with the updated scale lengths and scale length laws and found a CN production rate law consistent with that of C_3 as determined by ATM. Both of these pointed to a dependence on the heliocentric distance consistent with an inverse square law out to the $r_H \sim 2.5$ AU. The case for C_2 , on the other hand has been different.

ATM had assumed both C_2 and CN parent scale lengths varying as r_H^{+1} . Subsequent papers (A'Hearn et al., 1979, A'Hearn and Cowan, 1980 and A'Hearn and Millis, 1980) have used this same scale length law for C_2 , but have now used our revised values for CN. In Table 3 we present the re-reduced C_2 and CN production rates, assuming the new Haser scale length laws as well as the corrected g-factor for $C_2(0-0)$ (i.e., 4.5×10^{-13} ergs s^{-1} per radical, A'Hearn 1985).

The production rates for both C_2 and CN in Comet West now vary almost exactly as r_H^2 . The steep drop off in C_2 production rate from an r_H^2 law for $r_H > 1.5$ AU has been eliminated. A plot of the C_2 /CN ratio versus r_H for Comet West is shown in Figure 7. A'Hearn and Millis (1980) had found that this apparent relative depletion of C_2 at larger heliocentric distances has been found in many comets, both periodic and new. A'Hearn and Cowan (1980) had attributed this to the hypothesis that the C_2 parent is embedded in grains of a less volatile component than water whose vaporization turns off at a higher temperature than the bulk vaporization of the nucleus. They have

constructed a model which quantitatively explains the data. This explanation now no longer seems necessary.

We have also re-reduced all of the photometry of six comets, observed by A'Hearn and Millis (1980) for C_2 and CN, and find similar results. The values of the ratios of the production rates have been categorized in a way similar to that done by A'Hearn and Millis, in two groups: those with a heliocentric distance less than 1.5 AU and those greater than 1.5 AU. These results are summarized in Table 4. Using the old scale length laws, a sizeable depletion (45%) of C_2 relative to CN for $r > 1.5$ AU was found as in the case for Comet West, but with the revised scale length laws this depletion again disappears.

Thus we have explained the apparent drop of C_2 production rate for larger heliocentric distance to be simply an artifact of an inappropriate Haser scale length law.

V. RADIATION PRESSURE ON C_2

In Paper III, Combi (1980) had shown that the difference between the sunward and anti-sunward brightness profiles of a cometary radical due to solar radiation pressure could be quantitatively modeled and used to disentangle the velocity and lifetime from the decay scale length. The same many-particle Monte Carlo coma model has been used to analyze the profiles of C_2 as was used in Paper III for CN.

The model discussed in detail in Paper I (Combi and Delsemme 1980a) correctly models photochemical kinematics by taking into account the isotropic ejection of the daughter radicals. In the model, the trajectories of many radicals (usually 10^5) are actually calculated and the column and space densities are found by counting the number of radicals in grids of bins of known area and volume respectively. This is in contrast to the usual cometary free flow models which compute densities by numerical integration of emission flux functions.

Haser's model can be fitted to data in terms of three independent parameters: the ratio of Q (production rate) to v (radial outflow speed), and the two scale lengths (one for production and one for decay of the daughter radical). In contrast, the Monte Carlo PTM without radiation pressure (and the vectorial model), owing to the isotropic ejection directions of daughter radicals, introduces two extra free parameters, which are the parent outflow and the radial ejection speeds. However, if a sizeable radiation pressure acceleration is present and can be independently calculated, and the distorted coma can be observed, the two additional parameters become constrained. Therefore, if one can determine the radiation pressure acceleration from the total solar fluorescence efficiency (g -factor) and can measure sunward and

antisunward brightness profiles (or a 2-dimensional mapping), then the velocities and lifetimes can be completely deconvolved.

The response of modeled sunward and antisunward profiles to the relative speeds of the radical and the parent is illustrated in Figure 8. The location of the sunward limit is set approximately by the maximum radial speed, v_{\max} (i.e., the scalar sum of the parent and radical ejection speeds), and the radiation pressure acceleration, a , as a $v_{\max}^2/2a$ envelope. The distance from the nucleus where the sunward and antisunward profiles diverge is set by the relative parent outflow and the radical ejection speeds. All three sets of model profiles in Figure 8 have the same radial (Haser) scale lengths, with the appropriate lifetimes being set using the ARWM. They also have the same sunward limit set by the maximum velocity and the acceleration. As radical speed increases, the location where the two profiles diverge moves back toward the nucleus.

The radiation pressure on a C_2 radical at 1 AU can be calculated from the fluorescence efficiency of the (0-0) band of the Swan System (4.5×10^{-13} ergs s^{-1} , A'Hearn 1975) and the observed relative band ratios for the rest of the system (A'Hearn 1985). We find a value of 0.81 cm s^{-2} . However, there is a large uncertainty in the absolute g -factor which may be as large as 40% (A'Hearn 1985). An alternate approach to constraining the model parameters would be to adopt the parent outflow speed law of Delsemme (1982).

From the compilation of halo expansion velocities measured by Bobrovnikov (1954) and Beyer (1961), Whipple (1980) has suggested that the initial radial velocity of parent molecules expanding from the nucleus is given approximately as $0.535 r_H^{-0.6}$ in km/sec where r_H is the comet's heliocentric distance. Delsemme (1982) has added to this data set the result of Malaise (1970) who deduced outflow velocities near the nucleus using the Swings-Greenstein effect on CN rotational lines. Furthermore, Delsemme has provided a simple

theoretical argument that, since a temperature law of $T = T_0 r_H^{-1}$ is expected, the true radial velocity expansion law should now be given as

$$v = (.58 \pm .03) r_H^{-0.5}.$$

The change in the power law exponent is due to the fact that Bobrovnikov's and Beyer's data beyond 3 AU must clearly reflect vaporization of gases more volatile than water; the constant shift corresponds to a factor of 1.25, yielding an average molecular weight of 28 for these gases. Either CO or a mixture of CO₂ with lighter gases could explain this shift.

If we adopt this parent speed law, then the best fit models to the observed profiles will yield both lifetimes, the radical outflow speed and the radiation pressure acceleration. It was found that the best fits to all three of the pairs of C₂ profiles (shown as the solid lines in Figures 2, 3 and 4) in Comet Bennett were obtained with an ejection velocity of $\sim 0.5 \text{ km s}^{-1}$. The corresponding profiles for the limited Comet Kohoutek profiles have also been calculated and are shown in Figure 5. The numerical results of the Monte Carlo PTM analysis of the three pairs of C₂ profiles in Comet Bennett are summarized as follows:

Assumptions:

- (1) $v \text{ (parent)} = 0.58/r^{1/2} \text{ km/s}$
- (2) $C_2X + h\nu \rightarrow C_2 + X + (\text{Energy})$

Results at 1 AU:

$$\begin{aligned} v_e (C_2) &= 0.5 \text{ km/s} \\ \tau \text{ (parent)} &= 3.1 \times 10^4 \text{ s} \\ \tau \text{ (daughter)} &= 1.2 \times 10^5 \text{ s} \\ a \text{ (rad. pr.)} &= 0.70 \text{ cm/s}^2 \end{aligned}$$

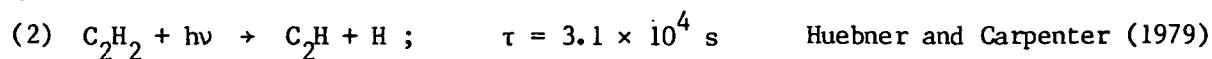
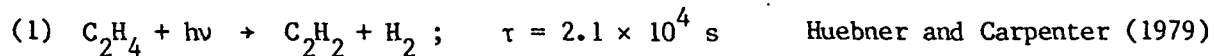
A value for the radiation pressure acceleration of 0.70 cm s^{-2} , found from the model analysis, compares rather favorably with the value calculated from the g-factor (0.81 cm s^{-2}). In fact, this is well within the 40% uncertainty expected for the g-factor. The self consistency in the results lends confidence in the model, the g-factor and a parent outflow speed of $\sim 0.6 \text{ km s}^{-1}$ near 1 AU. Of course, since we have observations over only a narrow range of heliocentric distance (0.84 to 1.0 AU), we really can neither confirm nor deny the validity of the Delsemme velocity law.

VI. POSSIBLE SOURCES OF C₂

We now turn to the question of examining the possible C₂ source(s) in comets in terms of the deduced production lifetime (i.e., destruction of the parent) found to be $\sim 3.1 \times 10^4$ s at $r_H = 1$ AU and the ejection speed of 0.5 km s^{-1} . The uncertainty in this lifetime can be crudely estimated from the uncertainties in the (0-0) band g-factor (40%), the parent velocity law (6%), and the effective scale length fitting procedure ($\lesssim 15\%$). Since the spatial distortion is in effect set by a $\frac{v^2}{2a}$ paraboloid envelope, uncertainties in the inferred velocities enter as the square root of those in the radiation pressure acceleration (the g-factor). Therefore, a total uncertainty of $\sim 20\%$ in the determined parent lifetime is expected if one relies on the parent velocity law and of $\sim 35\%$ if one relies on the g-factor.

C₃ once seemed like a viable candidate for at least a major source of cometary C₂, but the g-factor for the 4040 Å band has been revised upward by a factor of 40 (A'Hearn 1982). Thus, the C₃ production rate is now believed to be nearly two orders of magnitude less than C₂ and CN.

In their extensive work on solar photochemical radiation rates, Huebner and Carpenter (1979) had calculated the photochemical lifetimes of C₂H₂ and C₂H₄. The following reactions which may ultimately produce C₂, shown with the lifetime of the original reactant, are:



It seems that with a total parent lifetime of 3.1×10^4 s found in this paper (i.e., total meaning all steps of multiple step process added up to yield a simple effective parent lifetime), C_2H_4 can probably be eliminated as a principal parent. Furthermore, even C_2H_2 would only be possible if the lifetime for reaction (3) were very short. This would be precisely the same conclusion reached with the chemical model by Cochran (1985a), who placed a value of 2000 s on the lifetime for C_2H in order for acetylene to be the primary parent frozen in the cometary nucleus. However, new information regarding the C_2H_2 photodissociation has become available (Huebner 1985) which revises the lifetime of C_2H_2 upward (or the reaction rate downward) by more than factor of two. These new data are given in Table 6. The reaction rate for photodissociation of the C_2H radical is still unknown. A photochemical lifetime of 7.9×10^5 s and the large ejection speeds would appear to eliminate C_2H_2 as the only or principal primary parent for C_2 .

However, the determination of photodissociation rates from solar spectral fluxes and laboratory-measured photoabsorption cross sections is not a simple problem. Even in cases where a complete absorption spectrum has been measured, the validity of this approach is complicated by (1) the multiline nature of the solar UV spectrum, (2) the relatively low wavelength resolution of the experiments (~ 10 Å) and, most importantly, (3) the high density and high internal temperature (~ 270 K) of the target gas. As cometary molecules leave the collisionally dominated inner region, they naturally undergo rapid radiative cooling, leaving them in their lowest rotational and vibrational levels ($T < 100$ K). Actual photodissociation cross sections (and the major branching ratios) can be more than two orders of magnitude different from those values measured in the laboratory (Jackson 1982).

These difficulties can be best illustrated by the widely varying total solar photorates quoted for C_2H_2 over the years in the literature: 1.6×10^5 s by Potter and DelDuca (1964); 5.7×10^3 s by Jackson (1976); 3.1×10^4 s by Huebner and Carpenter; and 7.9×10^4 s by Huebner (1985). Finally, Huebner (1985) has suggested that C_2 may be produced by a combination of many sources, possibly including C_2H_2 . In any event, the effective lifetime of the C_2 source(s) has been determined empirically here to be $\sim 3.1 \times 10^4$ s.

The case for attempting to identify the parent(s) of cometary C_2 is a perfect example of the dangers in trying to use complicated chemical models for routine analyses of observed spatial distributions of cometary radicals. Revisions by factors of 2 to 5 are to be expected as better laboratory measurements and ab initio calculations of gas phase chemical and photochemical reactions are made. In this case, a revision by a factor of 2.5 in only one out of >1000 reactions completely reversed an interpretation. (Furthermore, the same interpretation would have been drawn using the old reaction rate and the Haser and Monte Carlo model approach adopted in this paper.)

VII. SUMMARY

1. Brightness profiles of C_2 in Comets Bennett (1970II) and Kohoutek (1973XII) have been presented.
2. Radial (Haser) scale lengths for production and destruction of C_2 have been determined from these profiles, and when compared with those determined from other brightness profiles in the literature are found to be consistent with both scale lengths varying as the square of the heliocentric distance (r). An updated compilation of the CN Haser scale lengths yields an $r^{1.5}$ for the CN parent.
3. The production rates of C_2 and CN as determined from the photometry of A'Hearn et al. (1977) and A'Hearn and Millis (1980) have been recalculated using Haser's model and the new scale length r -dependences. The drop in production rate of C_2 relative to CN (and presumably other species) for heliocentric distances >1.5 AU is now eliminated. Furthermore, the production rates of both C_2 and CN in Comet West vary almost precisely as the inverse square of the heliocentric distance.
4. Monte Carlo particle-trajectory models which take into account the radiation pressure acceleration on C_2 were fitted to the sunward and antisunward pairs of profiles for Comet Bennett. These results yield a photochemical lifetime of 3.1×10^4 seconds of 1 AU for the parent(s) of C_2 and an ejection velocity of $\sim 0.5 \text{ km s}^{-1}$ for C_2 upon dissociation and a radiation pressure acceleration consistent with that expected for solar fluorescence, if one assumes a parent outflow of $\sim 0.6 \text{ km s}^{-1}$ (Delsemme 1982). A photochemical lifetime of 1.2×10^5 seconds for C_2 was found.

This interpretation is consistent with the radiation pressure acceleration as determined by the total C_2 solar fluorescence rate.

5. We have examined the possible molecular sources for cometary C_2 in terms of the parent lifetime of 3.1×10^4 seconds at 1 AU. C_2H_4 in a multiple step process seems unlikely as an ultimate source. C_2H_2 as the sole or even primary source is also inconsistent with the recently updated photodissociation rates for C_2H_2 (Huebner 1985).

Acknowledgments

The authors would like to thank Drs. W.F. Huebner and A.L. Cochran for helpful discussions. Work at AER was supported under NASA contract NASW-3950. Work at the University of Toledo was supported in part by grants ASY 82-07435 from NSF and NSG-7301 from NASA.

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TABLE 1

Observational Data

Comet	UT	r^a (AU)	Δ^b (AU)	ϕ^c
Kohoutek (1973XII)	January 9.11, 1974	.465	.846	85.5°
Bennett (1970II)	April 18.4, 1970	.841	1.054	62.5°
Bennett (1970II)	April 26.4, 1970	.970	1.247	51.8°
Bennett (1970II)	April 27.4, 1970	.986	1.271	50.7°

^a heliocentric distance

^b geocentric distance

^c sun-comet-earth angle

TABLE 2
C₂ Scale Lengths from Haser's Model

<u>Observers</u>	<u>Comet</u>	<u>r_H (AU)</u>	<u>$\log \gamma_{PH}$ (km)</u>	<u>$\log \gamma_{dH}$ (km)</u>
O'Dell and Osterbrock (1962)	Burnham (1960II)	1.00	-	4.93
Delsemme and Miller (1971)	Burnham (1960II)	1.00	4.10 ^b	4.95
Kumar and Southall (1976)	Tago-Sato-Kosaka (1969IX)	1.25	4.40	5.09
Malaise (1976) ^a	Bennett (1970II)	0.664	3.61	4.83
Malaise (1976) ^a	Bennett (1970II)	0.713	3.95	5.08
Cochran (1985)	P/Tuttle	1.019	4.25 ^b	5.11 ^b
Cochran (1985)	P/Stefan-Oterma	1.58	4.62 ^b	5.68 ^b
Cochran (1985)	Meier	1.755	4.72 ^b	5.59 ^b
this work	Kohoutek (1973XII)	0.465	3.69	4.29
this work	Bennett (1970II)	0.841	4.05	4.78
this work	Bennett (1970II)	0.970	4.08	4.97
this work	Bennett (1970II)	0.986	4.23	4.92

^a Scale length was computed by Combi (1978) from the original data.

^b Determined from the data for this paper.

TABLE 3

Production Rates of C_2 and CN in Comet West (1976VI)

<u>r (AU)</u>	<u>$\log Q_{C_2}(s^{-1})^a$</u>	<u>$\log Q_{CN}(s^{-1})^a$</u>
0.468	27.675	27.707
0.522	27.662	27.790
0.522	28.757	27.782
0.522	27.664	27.733
0.600	27.483	27.495
0.651	27.560	27.567
0.773	27.295	27.340
0.820	27.432	27.426
0.889	27.206	27.208
1.044	27.203	27.129
1.406	26.665	26.640
1.443	26.535	26.645
1.443	26.544	26.625
1.554	26.688	26.722
1.767	26.738	26.814
1.852	26.683	26.837
1.852	26.666	26.844
2.002	26.439	26.604
2.146	26.417	26.554
2.209	26.157	26.403
2.497	26.255	26.182
2.540	26.097	26.243
2.550	26.281	26.388

^a Recalculated from the photometry of A'Hearn et al. 1977 with the new revised Haser scale length laws.

TABLE 4

Production Rates of C₂ and CN in Six Comets

<u>r (AU)</u>	<u>log Q_{C₂}(s⁻¹)^a</u>	<u>log Q_{CN}(s⁻¹)^a</u>
P/Ashbrook-Jackson (1978XIV)		
2.349	25.31	-
2.347	24.92	25.05
2.344	25.02	24.79
2.288	24.95	24.74
P/Wild 2 (1978XI)		
1.803	25.19	25.18
1.497	25.62	25.44
1.495	25.63	25.49
1.495	25.64	25.43
1.493	25.62	25.42
1.493	25.68	25.48
Meier (1978XXI)		
2.858	26.72	25.57
2.587	26.93	26.69
2.553	27.00	26.73
2.553	27.14	26.73
2.222	<25.15	26.79
2.211	-	26.82
P/Haneda-Campos (1978XX)		
1.177	24.26	23.88
Bradfield (1979c)		
0.960	24.83	24.84
0.978	24.84	24.88
Meier (1979i)		
1.479	25.19	24.87

^a Recalculated from the photometry of A'Hearn and Millis (1980) with the new revised Haser scale length laws.

TABLE 5

Q(C₂)/Q(CN) Ratio for Six Comets

$\log \frac{Q(C_2)}{Q(CN)}$	Current ^(a) Scale Lengths	New Scale Lengths
$r < 1.5 \text{ AU}$	+0.072	+0.176
$r > 1.5 \text{ AU}$	-0.088	+0.178

(a) A'Hearn and Millis (1980, A.J. 85, 1528)

TABLE 6
C₂H₂ Photochemistry

	Rate ^a (s ⁻¹)	E _{excess} ^a (eV)	v _{heavy} (km s ⁻¹)	
C ₂ H ₂ + hν → C ₂ H + H	1 × 10 ⁻⁵	3.2	0.97	79%
→ C ₂ + H ₂	2.7 × 10 ⁻⁶	3.1	1.4	21%

$$\tau (\text{C}_2\text{H}_2) = 7.9 \times 10^4 \text{ s} \quad (\text{previous value} = 3.2 \times 10^4)$$

$$\tau (\text{C}_2\text{H}) = \text{still unknown}$$

^aHuebner (1985)

FIGURE CAPTIONS

- Figure 1. Variation of CN Haser Parent (a) and Daughter (b) Scale Length with Heliocentric Distance. The points show the values which result from Haser model fits to whole brightness profiles. In (a) the line shows the best fit power law of $1.6 \times 10^4 r_H^{1.5}$ km. In (b) the daughter scale lengths exhibit no obvious trend but likely reflect only coma activity (Combi and Delsemme 1980b).
- Figure 2. Brightness Profiles of C_2 in Comet Bennett (1970II). The points show the data taken on April 18, 1970, and the solid lines show the best fit Monte Carlo particle-trajectory model with radiation pressure acceleration. The open circles are sunward and the filled circles are antisunward.
- Figure 3. Brightness Profiles of C_2 in Comet Bennett (1970II). The points show the data taken on April 26, 1970; see Figure 2 for explanations.
- Figure 4. Brightness Profiles of C_2 in Comet Bennett (1970II). The points show the data taken on April 27, 1970; see Figure 2 for explanations.

Figure 5. Brightness Profiles of C_2 in Comet Kohoutek (1973XII). The points marked sunward and antisunward are actually 51° from the true directions. Because of the limited spatial extension, especially sunward, no asymmetric profile information could be extracted. However, the corresponding Monte Carlo PTM (solid lines) were computed for this observational geometry with model parameters scaled appropriately from the other pairs of profiles.

Figure 6a. Variation of C_2 Haser Parent Scale Length with Heliocentric Distance. The points correspond to the values shown in Table 2. The lines show the best power law fit of $r_H^{2.0}$.

Figure 6b. Variation C_2 Haser Daughter Scale Length with Heliocentric Distance. The points correspond to the values shown in Table 2. The lines show the best power law fit of $r_H^{2.0}$.

Figure 7. Ratio of the Production Rates of C_2 to CN in Comet West (1976VI). The open squares correspond to the reduction of photometric band fluxes determined by A'Hearn et al. (1977) and reduced with the Haser scale lengths adopted by A'Hearn and Cowan (1980). The filled circles correspond to our reduction of the photometric band fluxes reduced with the new Haser scale length laws as presented in this paper.

Figure 8. Effects of Radical Ejection Velocity on the Modeled Radiation Pressure Asymmetry. Three pairs of profiles are shown as modeled with the Monte Carlo particle-trajectory model. All three exhibit the same symmetric radial scale lengths, as determined with the Average Random Walk Model, but have different velocity ratios of radical ejection to parent outflow. As the radical ejection velocity is increased, the location where the sunward and antisunward profiles diverge from one another moves backward toward the nucleus. This response yields an effective method for disentangling velocities and lifetimes from observed scale lengths.

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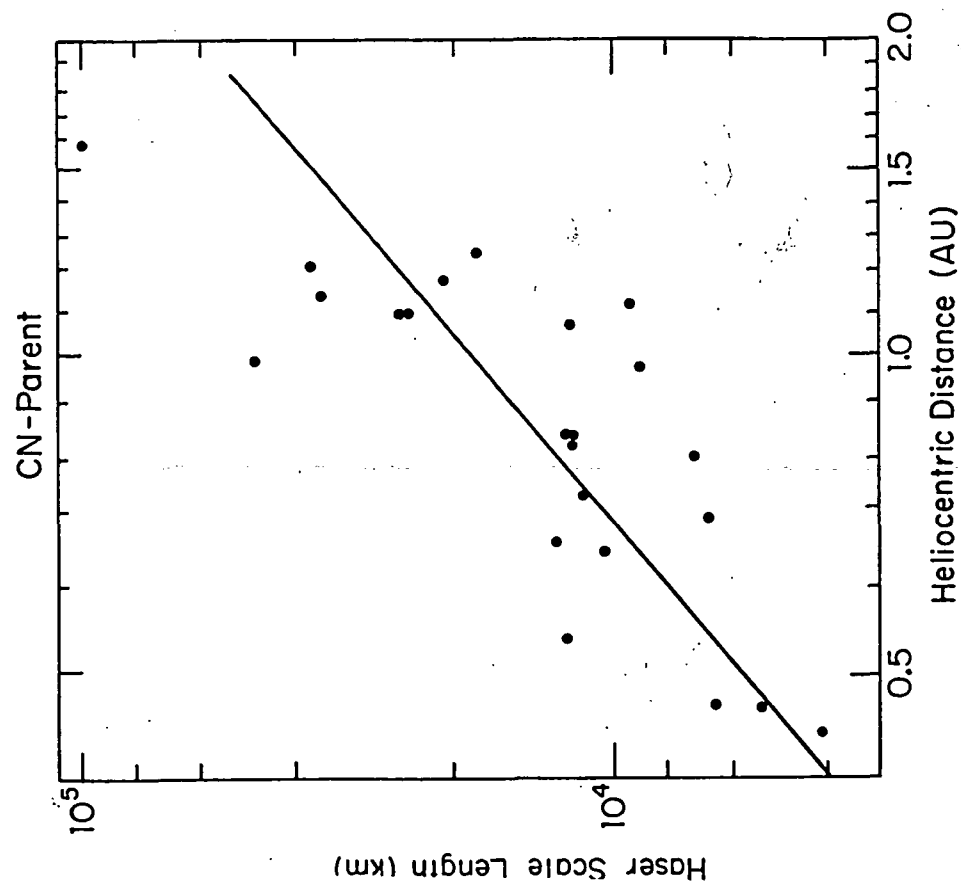


Figure 1a

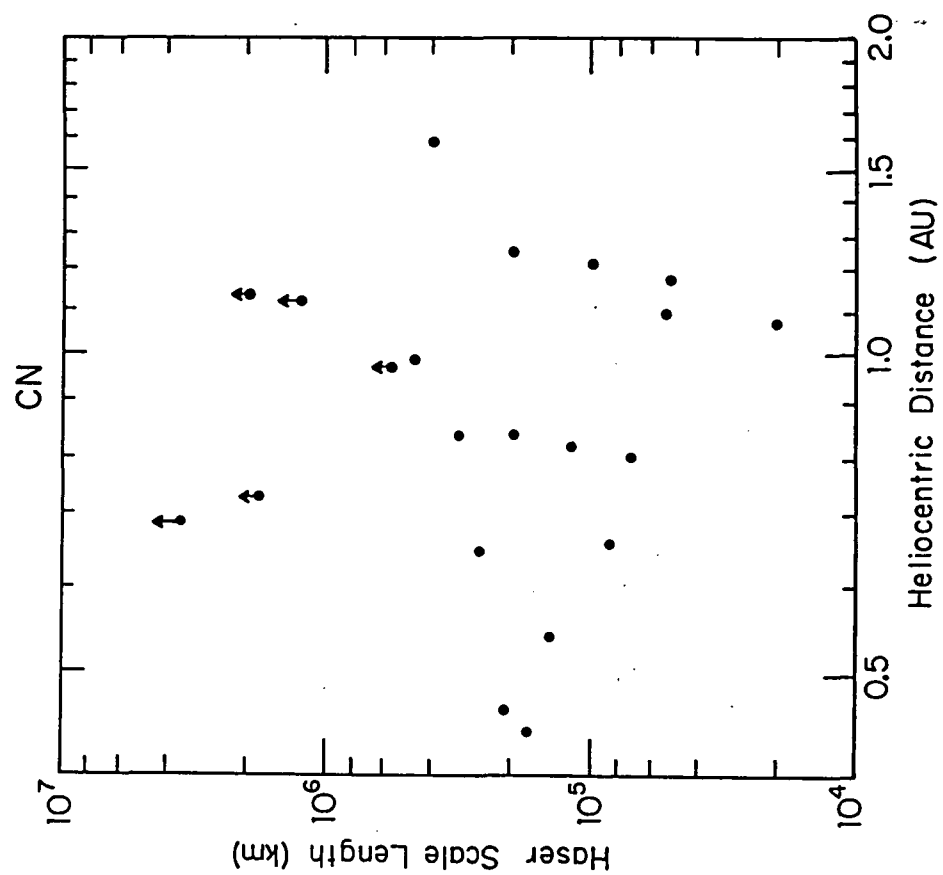


Figure 1b

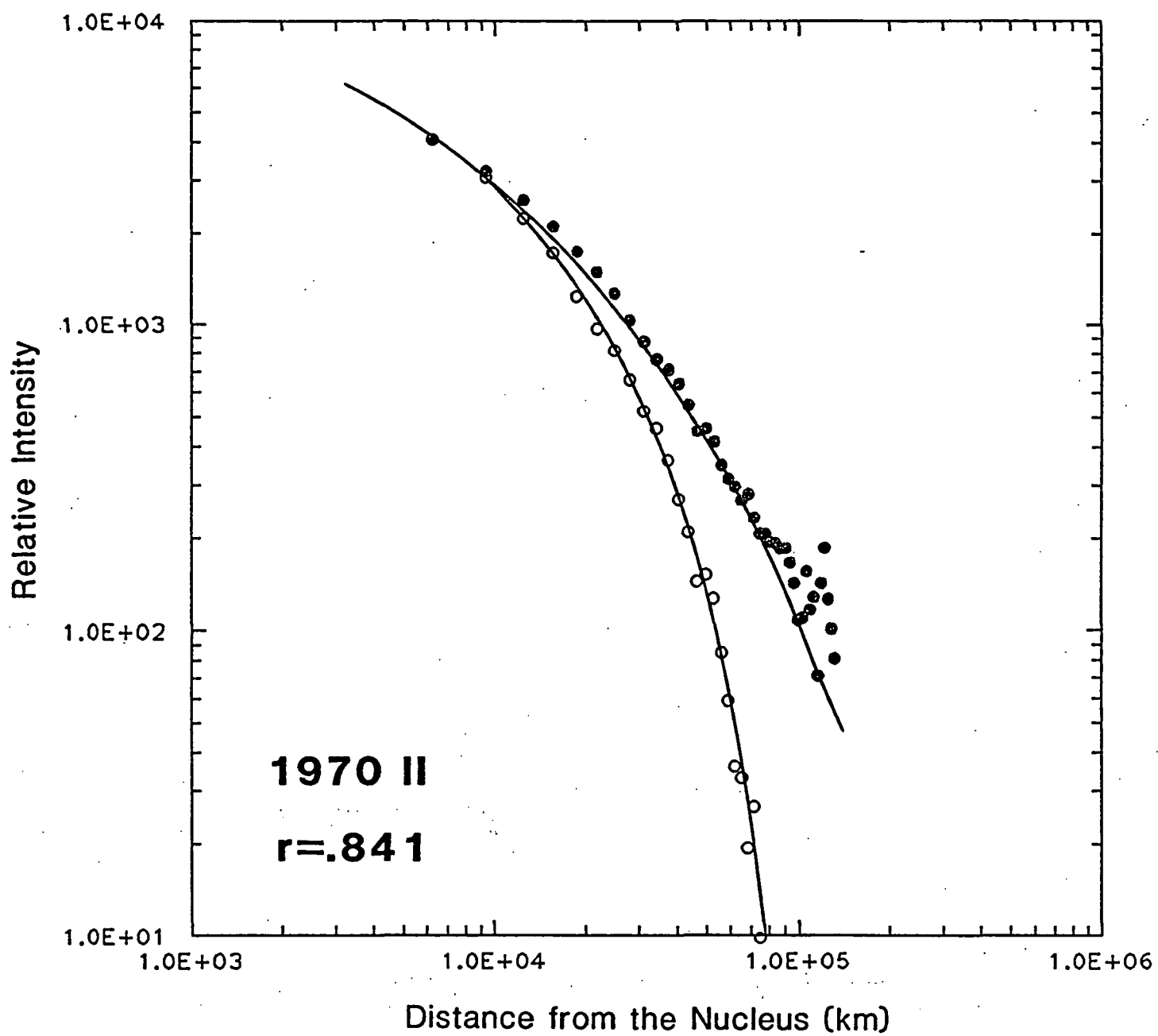


Figure 2

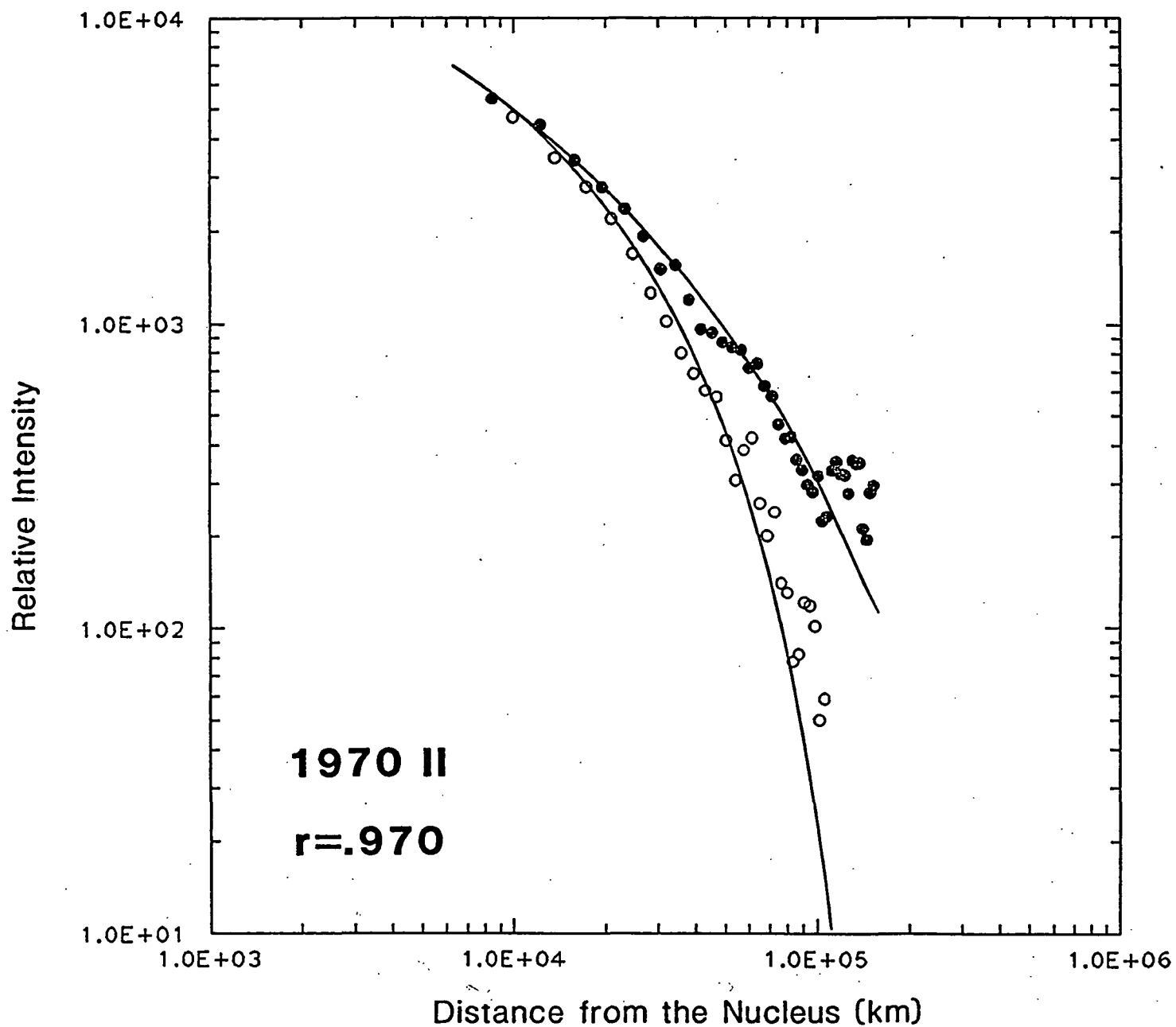


Figure 3

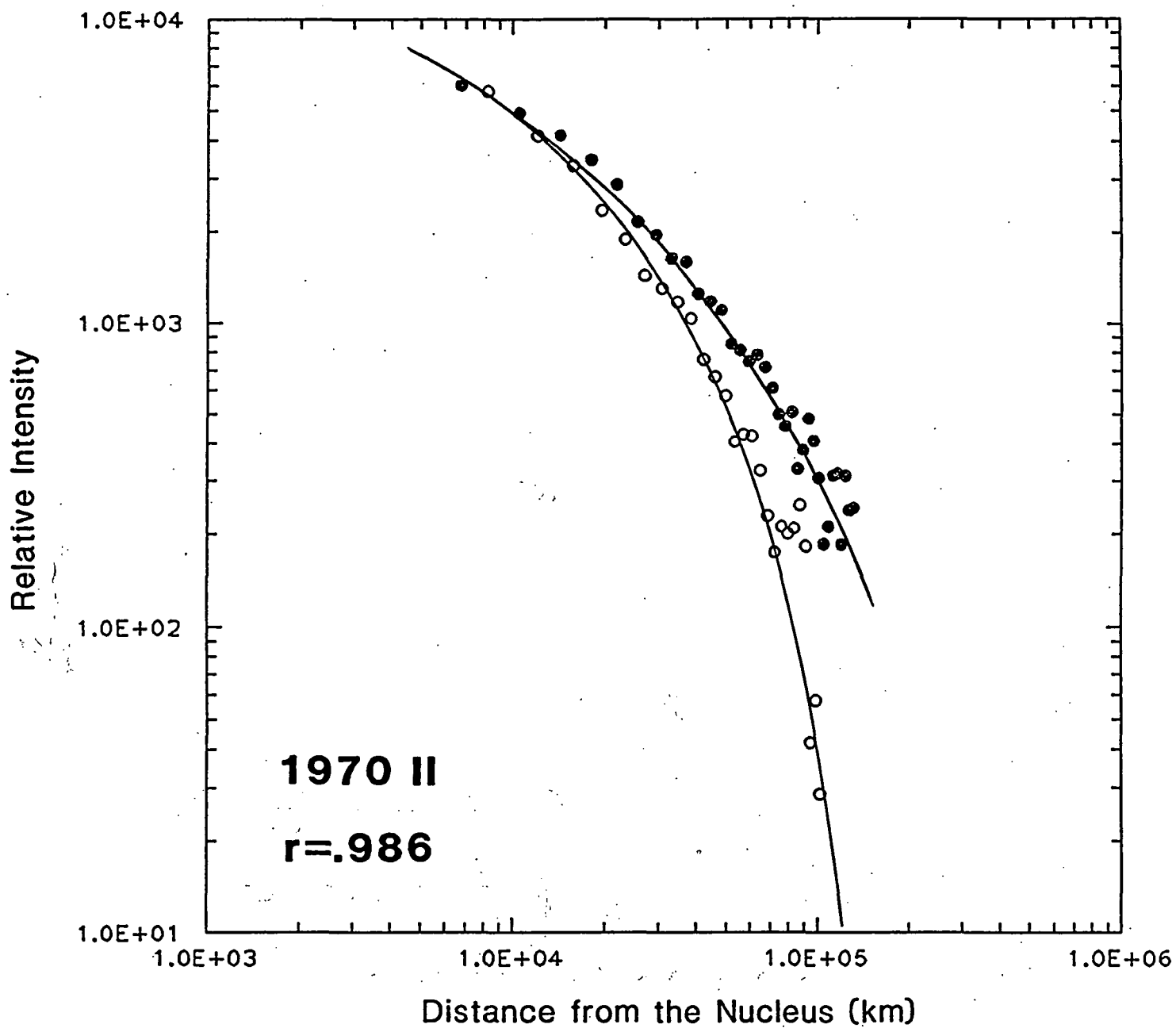


Figure 4

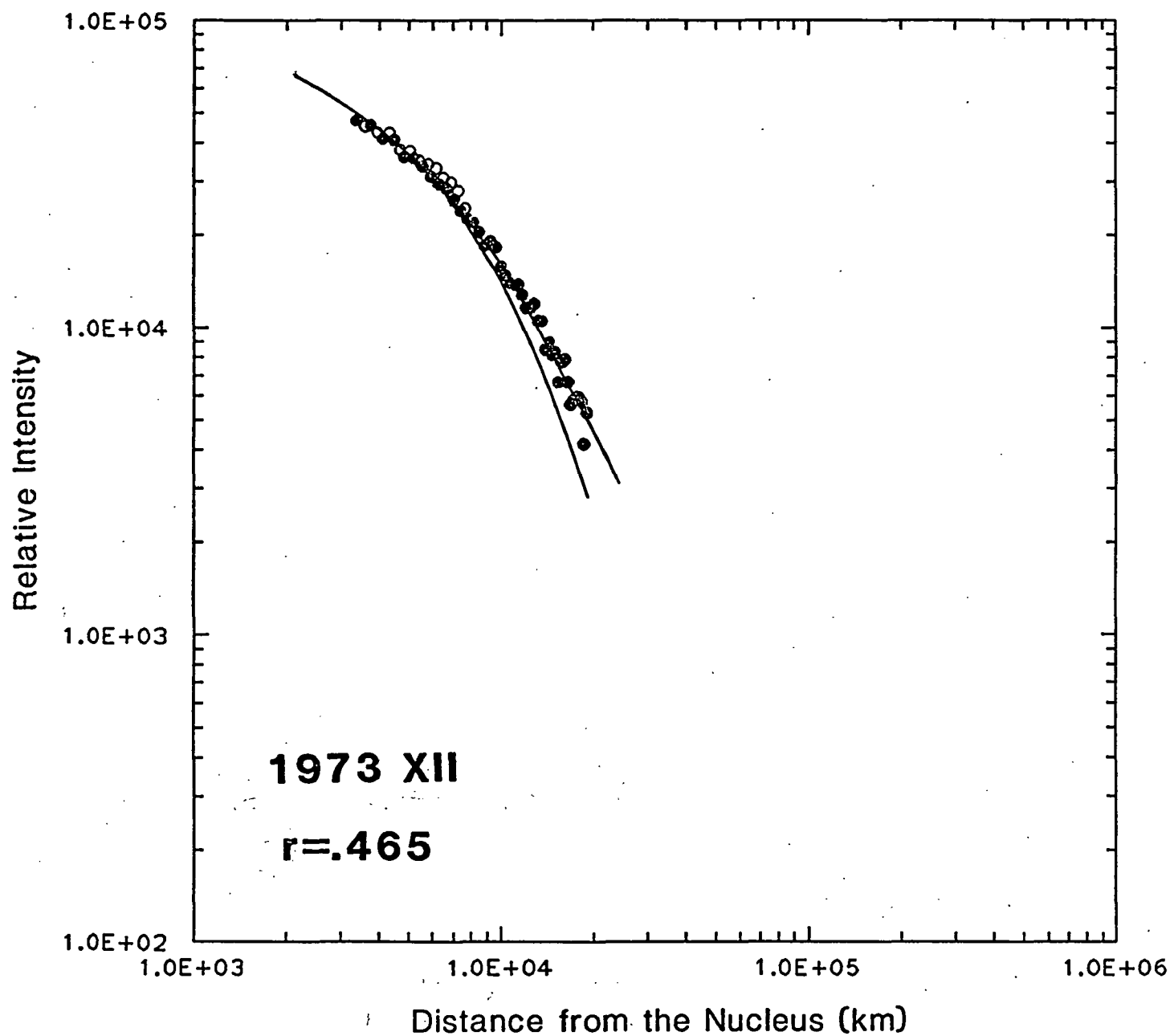


Figure 5

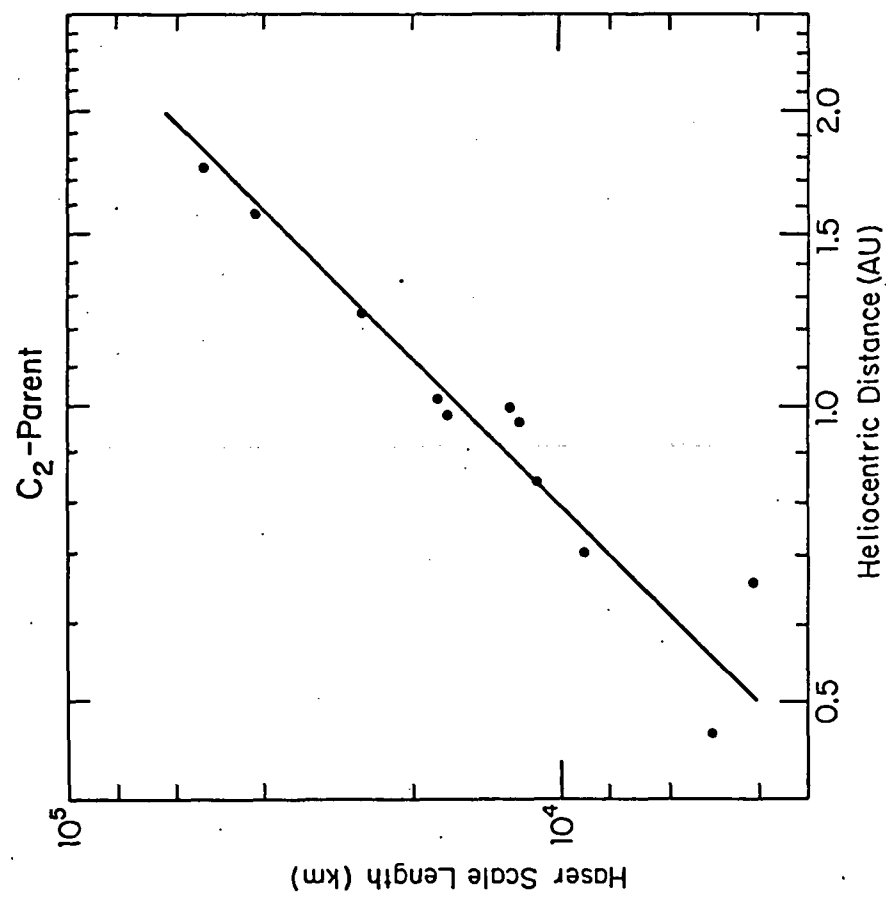


Figure 6a

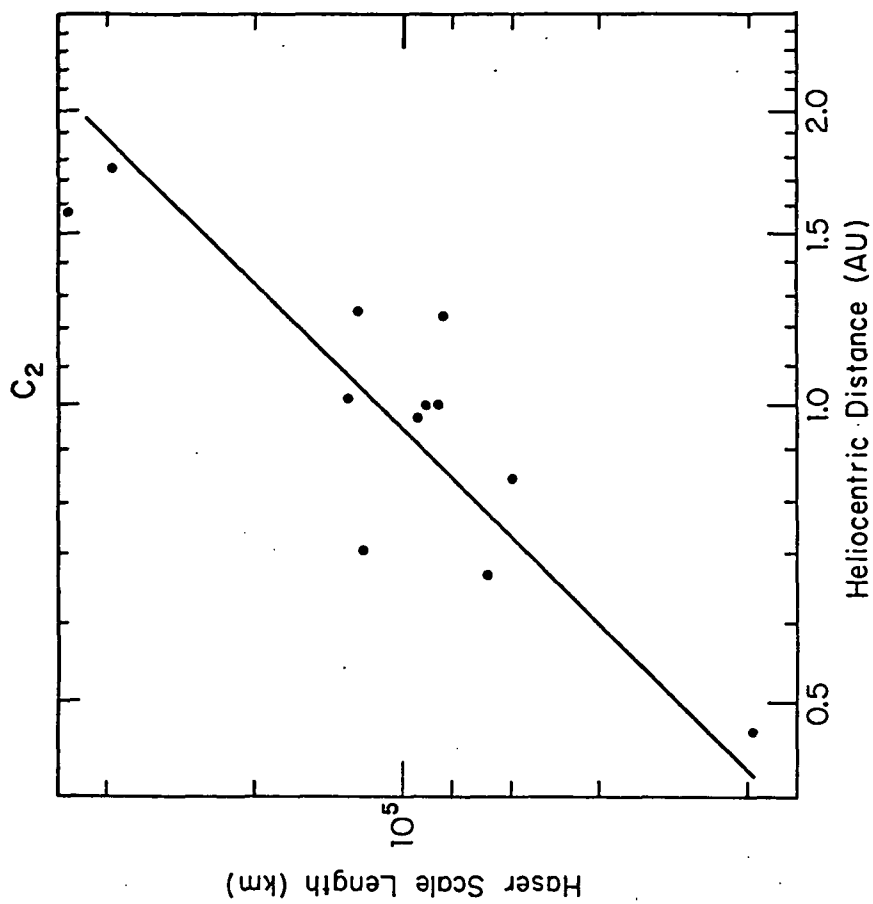


Figure 6b

C_2/CN Ratio in Comet West

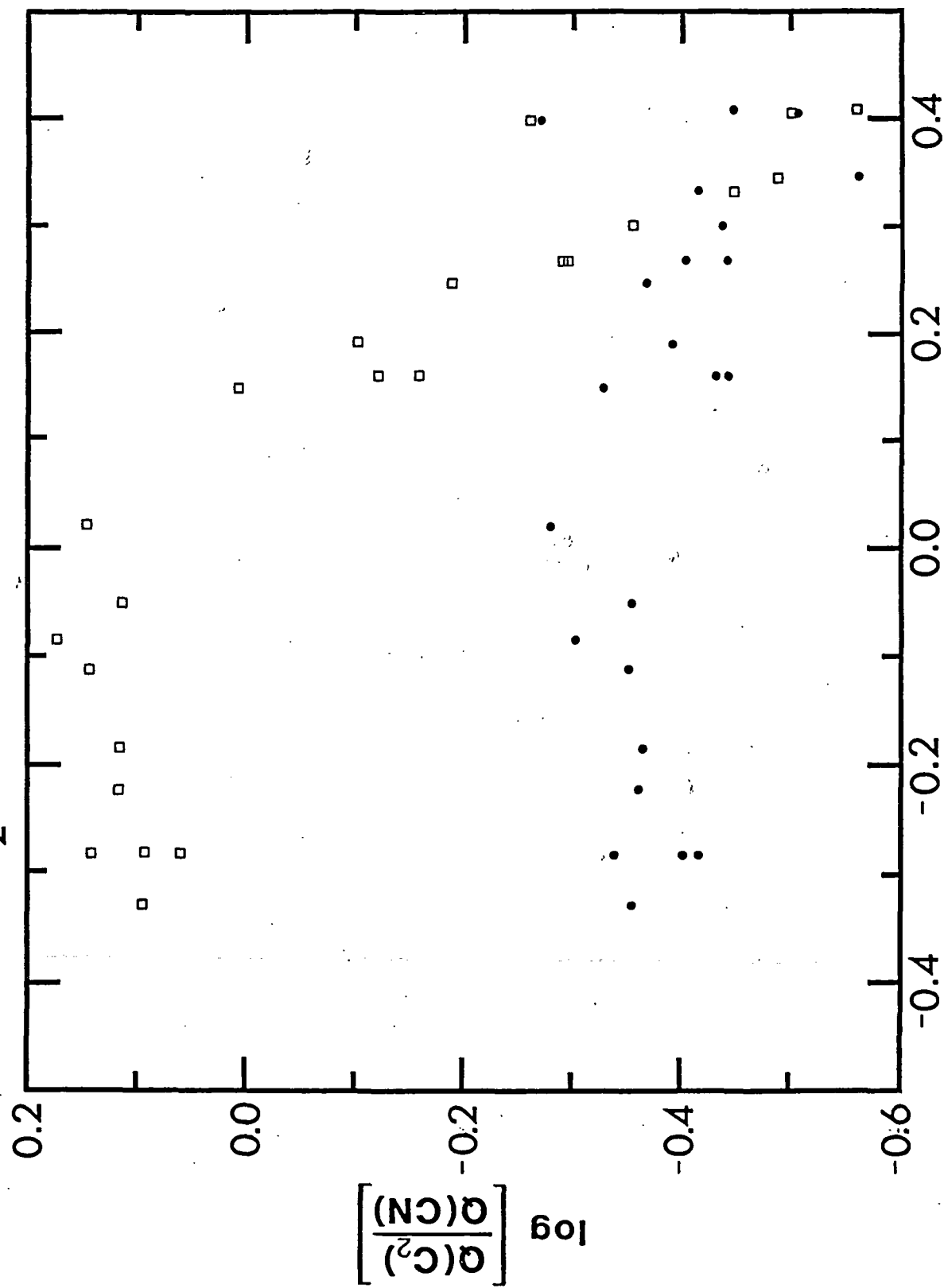


Figure 7

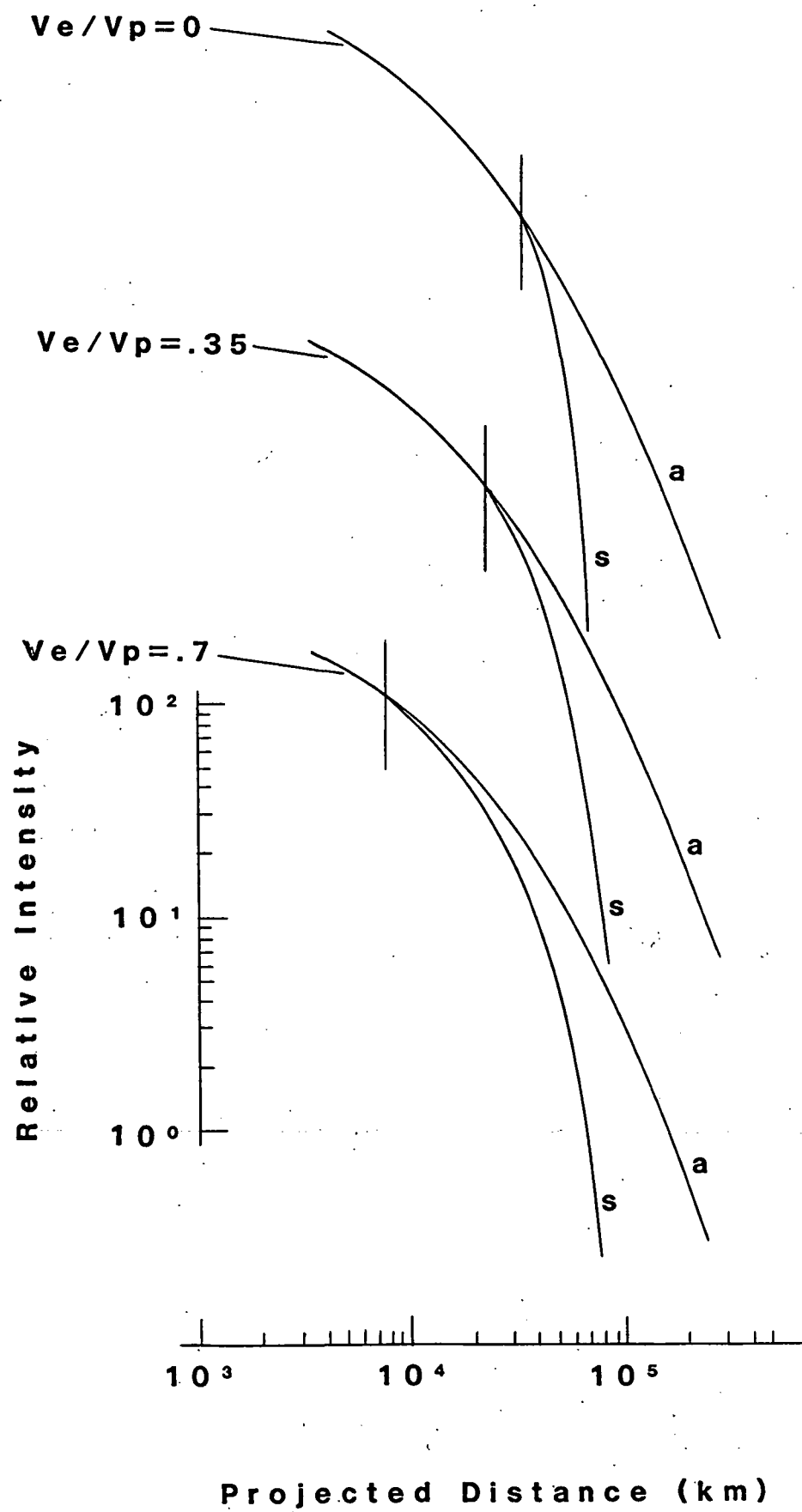


Figure 8